

# DFT analysis of magnetic properties of $L1_0$ $(\text{Fe}_{1-x}\text{Co}_x)\text{Pt}$ alloys for heat assisted magnetic recording

Wojciech Marciniak<sup>1,2</sup> and Joanna Marciniak<sup>1</sup>

<sup>1</sup>*Institute of Molecular Physics, Polish Academy of Sciences,  
M. Smoluchowskiego 17, 60-179 Poznań, Poland*

<sup>2</sup>*Institute of Physics, Poznań University of Technology,  
Piotrowo 3, 60-965 Poznań, Poland*

Constantly developing technology increases the demand for data carriers with increasingly high recording densities. This leads to the problem of maintaining the thermal stability of the recorded information, good signal-to-noise ratio, and recording fields small enough to be within the technologically available range. One way to circumvent this problem is to use materials with high perpendicular magnetic anisotropy together with the use of heat-assisted magnetic recording (HAMR) [1].

$L1_0$  FePt and CoPt phases are often considered in this context [2]. We showed previously that fine-tuning magnetic parameters of the  $L1_0$  FePt should be achievable [3]. In presented work, we investigate possible tailoring of magnetic properties of  $L1_0$  FePt by alloying with Co in the  $(\text{Fe}_{1-x}\text{Co}_x)\text{Pt}$   $L1_0$  phase in a lookout for any intermediate systems with better properties than the pure  $L1_0$  FePt and CoPt.

The calculations were performed using different density functional theory (DFT) codes: full-potential local-orbital (FPLO) and spin-polarized Korringa-Kohn-Rostoker (SPR-KKR) schemes. We compare several different implementations of the chemical disorder consideration, namely virtual crystal approximation (VCA) and coherent potential approximation (CPA) effective medium methods, supported by a direct Fe/Co full configuration space analysis in a  $2 \times 2 \times 2$  supercell. Due to the specificity of the utilized codes, we used the VCA and supercell methods in the FPLO code and the CPA method in the SPR-KKR code.

We present Co content dependencies of structural (unit cell volume, lattice constants ratio) and magnetic (magnetic moments, magnetocrystalline anisotropy energy (MAE)) properties of the system, as well as the MAE dependency on magnetic moment in the fixed spin moment (FSM) approach. We further evaluate changes in magnetic hardness and magnetostriction coefficient with Co concentration. In the disordered local moment (DLM) approximation, we calculate Curie temperatures in the SPR-KKR/CPA. The mixing enthalpy calculations for the full configuration space allows us to evaluate the overall stability of the system.

## References:

- [1] H. B. Luo *et al.*, J. Phys.: Cond. Matt. **26**(38) (2014) 386002
- [2] M. H. Kryder *et al.*, Proc. IEEE **96**(11) (2008) 1810-1835
- [3] J. Marciniak, W. Marciniak, M. Werwiński, J. Magn. Magn. Mater. **556** (2022) 169347

*We acknowledge the financial support of the National Science Centre Poland under DEC-2018/30/E/ST3/00267. The computations were, in the main part, performed on resources provided by the Poznan Supercomputing and Networking Center (PSNC). We thank Miroslaw Werwiński for valuable discussion, and Pawel Leśniak and Daniel Depcik for compiling the scientific software.*